



chain nodes :

23 24

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22

ring/chain nodes :

25 26 27 28

chain bonds :

7-25 10-26 11-24 14-23 15-28 18-27

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 12-15 13-14
13-18 15-16 16-17 16-19 17-18 17-22 19-20 20-21 21-22

exact bonds :

7-25 10-26 11-24 14-23 15-28 18-27

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 8-11 9-10 9-14 11-12 12-13 12-15 13-14
13-18 15-16 16-17 16-19 17-18 17-22 19-20 20-21 21-22

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:Atom 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS 28:CLASS